Optimization for Quantum Systems

Jeffrey Larson

Argonne National Laboratory

September 5, 2019

Quantum research with optimization

- Maximizing concurrence
- Improving ORBIT for stochastic functions
- Optimization of variational parameters
- Cutting quantum circuits
- Time-varying control

Maximizing concurrence

- Entanglement is the amazing (confusing) feature of quantum mechanics that motivates quantum research

Maximizing concurrence

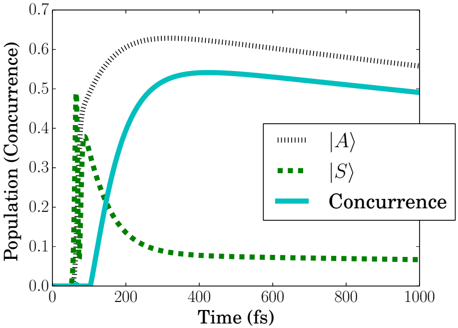
- Entanglement is the amazing (confusing) feature of quantum mechanics that motivates quantum research
- Concurrence is a measure of entanglement of a quantum system

Maximizing concurrence

- Entanglement is the amazing (confusing) feature of quantum mechanics that motivates quantum research
- Concurrence is a measure of entanglement of a quantum system
- Concurrence of two quantum dots excited by a single optical laser pulse:

Maximizing concurrence

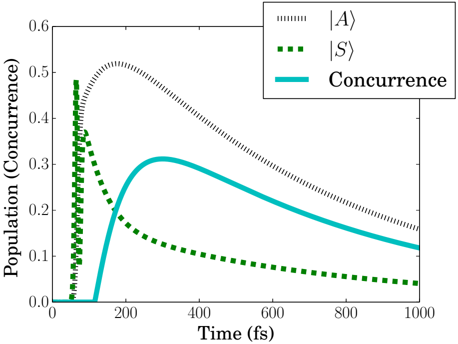
- Entanglement is the amazing (confusing) feature of quantum mechanics that motivates quantum research
- Concurrence is a measure of entanglement of a quantum system
- Concurrence of two quantum dots excited by a single optical laser pulse:



"QuaC: Parallel time Dependent Open Quantum Systems Solver." Otten

Maximizing concurrence

- Entanglement is the amazing (confusing) feature of quantum mechanics that motivates quantum research
- Concurrence is a measure of entanglement of a quantum system
- Concurrence of two quantum dots excited by a single optical laser pulse:



"QuaC: Parallel time Dependent Open Quantum Systems Solver." Otten

Maximizing concurrence

- Pairwise concurrence is measured by

$$C_{ij} = \max\{0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}\},$$

  where λ_k are the (descending) eigenvalues of a density matrix relating particles i and j.

Maximizing concurrence

- Pairwise concurrence is measured by

$$C_{ij} = \max\{0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}\},$$

  where λ_k are the (descending) eigenvalues of a density matrix relating particles i and j.
- Possible goal: Identify quantum system parameters x solving

Maximizing concurrence

- Pairwise concurrence is measured by

$$C_{ij} = \max\{0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}\},$$

  where λ_k are the (descending) eigenvalues of a density matrix relating particles i and j.

- Possible goal: Identify quantum system parameters x solving

Maximizing concurrence

- Pairwise concurrence is measured by

$$C_{ij} = \max\{0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}\},$$

  where λ_k are the (descending) eigenvalues of a density matrix relating particles i and j.

- Possible goal: Identify quantum system parameters x solving

$$\underset{x}{\text{maximize}} \sum_{ij} C_{ij}(x)^2$$

Maximizing concurrence

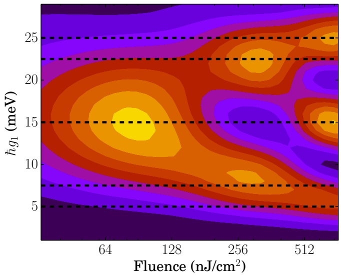
- Pairwise concurrence is measured by

$$C_{ij} = \max\{0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}\},$$

  where λ_k are the (descending) eigenvalues of a density matrix relating particles i and j.

- Possible goal: Identify quantum system parameters x solving

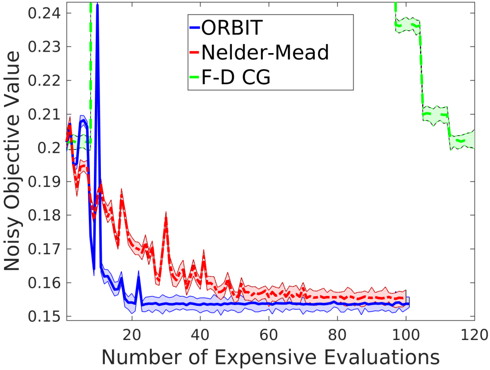
$$\underset{x}{\text{maximize}} \sum_{ij} C_{ij}(x)^2$$



Otten, Larson, Min, Wild, Pelton, Gray. Origins and optimization of entanglement in plasmonically coupled quantum dots. Physical Review A, 2016

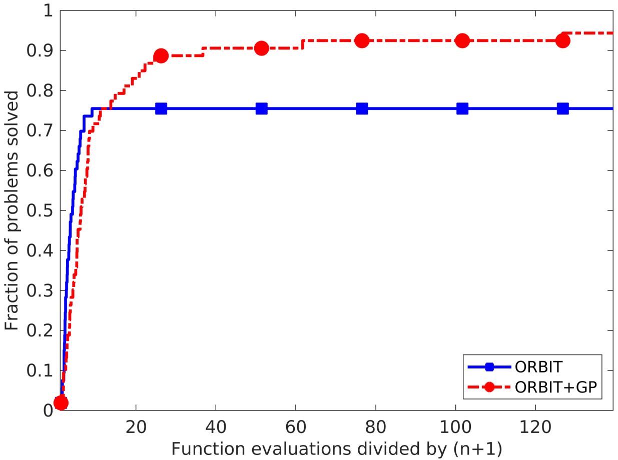
A 5D problem from Rigetti

Variational quantum eigensolver (VQE) methods want to identify the parameterization of the quantum state $|\psi\rangle$ at which $\mathbb{E}\left[H(|\psi\rangle)\right]$ is minimized.



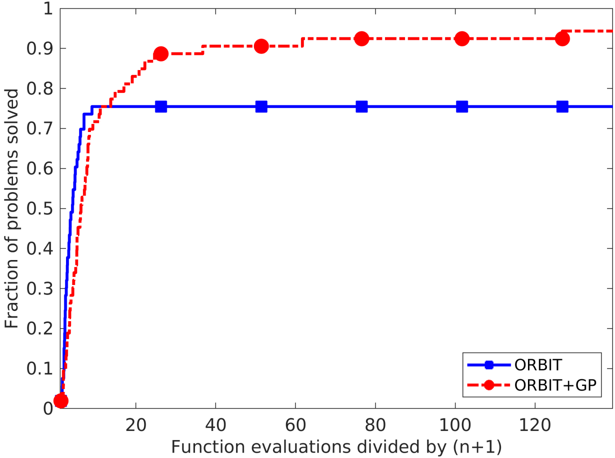
Wild, Shoemaker. Global convergence of radial basis function trust-region algorithms for derivative-free optimization. SIAM Review, 2013.

Improving ORBIT with Gaussian processes



53 stochastic benchmark problems with significant noise.

Improving ORBIT with Gaussian processes



"SKQuant-Opt: Optimizers for noisy intermediate-scale quantum devices", Lavrijsen, Tudor, Larson, Sung, Linder, Mueller, McClean, Babbush, Urbanek, Iancu, and de Jong, 2019

Quantum approximate optimization algorithm

- In QAOA, the quantum evolution starts in the initial state $|+\rangle^{\otimes n}$.

Quantum approximate optimization algorithm

- In QAOA, the quantum evolution starts in the initial state $|+\rangle^{\otimes n}$.

- The evolution is then performed by applying two alternating operators based on the cost Hamiltonian H_C and mixing Hamiltonian H_M

$$\begin{aligned} |\psi(\theta)\rangle &= |\psi(\beta,\gamma)\rangle \\ &= e^{-i\beta_p H_M} e^{-i\gamma_p H_C} \cdots e^{-i\beta_1 H_M} e^{-i\gamma_1 H_C} |+\rangle^{\otimes n}. \end{aligned}$$

Quantum approximate optimization algorithm

- In QAOA, the quantum evolution starts in the initial state $|+\rangle^{\otimes n}$.

- The evolution is then performed by applying two alternating operators based on the cost Hamiltonian H_C and mixing Hamiltonian H_M

$$\begin{aligned}|\psi(\theta)\rangle &= |\psi(\beta,\gamma)\rangle \\ &= e^{-i\beta_p H_M} e^{-i\gamma_p H_C} \cdots e^{-i\beta_1 H_M} e^{-i\gamma_1 H_C} |+\rangle^{\otimes n} .\end{aligned}$$

- p is the number of QAOA "steps."

Quantum approximate optimization algorithm

- In QAOA, the quantum evolution starts in the initial state $|+\rangle^{\otimes n}$.

- The evolution is then performed by applying two alternating operators based on the cost Hamiltonian H_C and mixing Hamiltonian H_M

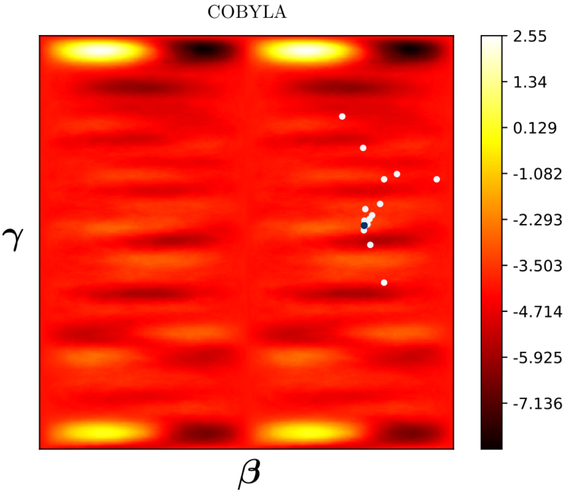
$$\begin{aligned} |\psi(\theta)\rangle &= |\psi(\beta, \gamma)\rangle \\ &= e^{-i\beta_p H_M} e^{-i\gamma_p H_C} \cdots e^{-i\beta_1 H_M} e^{-i\gamma_1 H_C} |+\rangle^{\otimes n} . \end{aligned}$$

- p is the number of QAOA "steps."

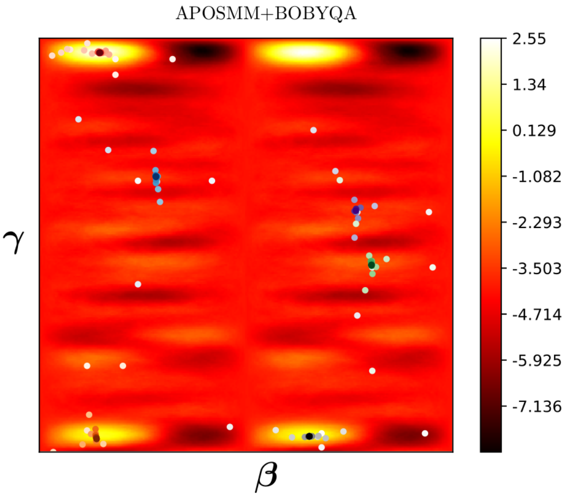
- Then the objective function f (i.e., the energy of H_C in the state $|\psi(\beta, \gamma)\rangle$) is

$$f(\beta, \gamma) = -\langle \psi(\beta, \gamma)| H_C |\psi(\beta, \gamma)\rangle .$$

QAOA on graph clustering

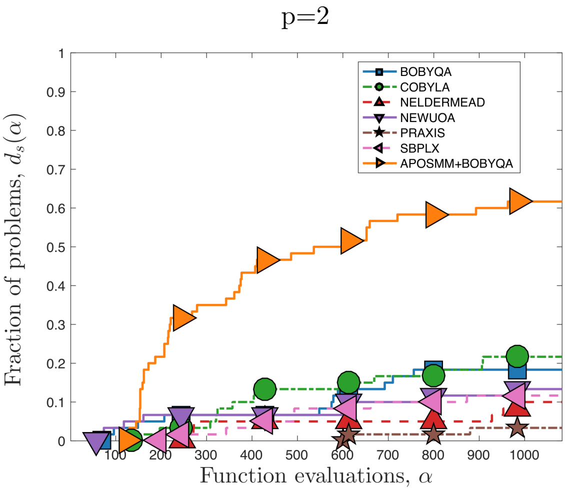


QAOA on graph clustering



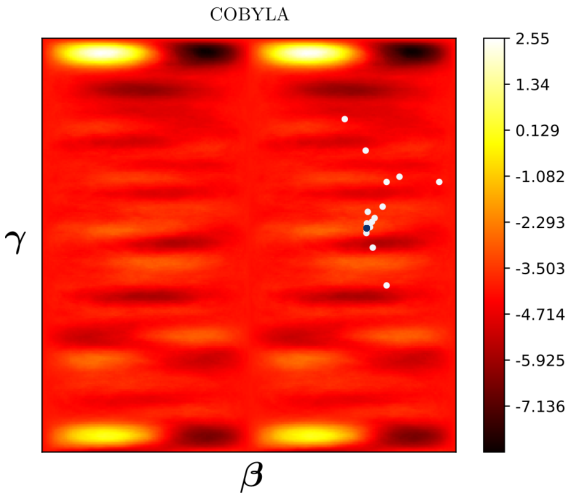
Larson, Wild. Asynchronously parallel optimization solver for finding multiple minima. Mathematical Programming Computation, 2018

QAOA on graph clustering



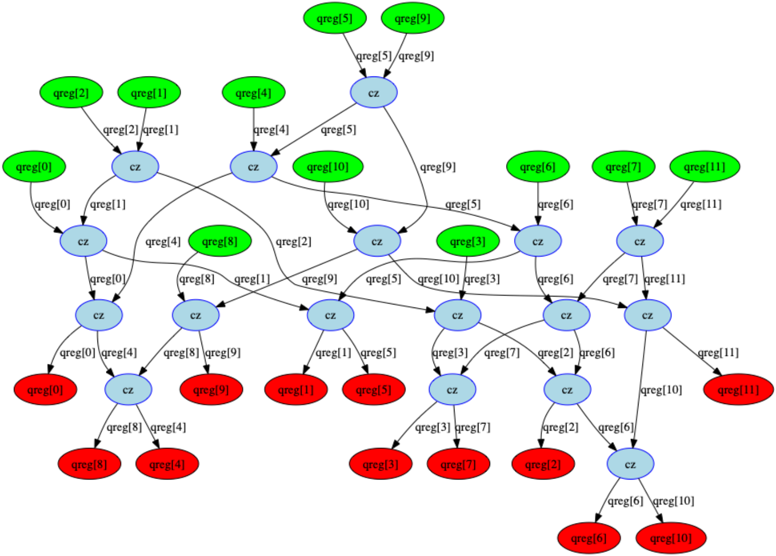
Shaydulin, Safro, Larson. Multistart Methods for Quantum Approximate Optimization. 2019 IEEE High Performance Extreme Computing Conference. (Best student paper finalist)

QAOA on graph clustering

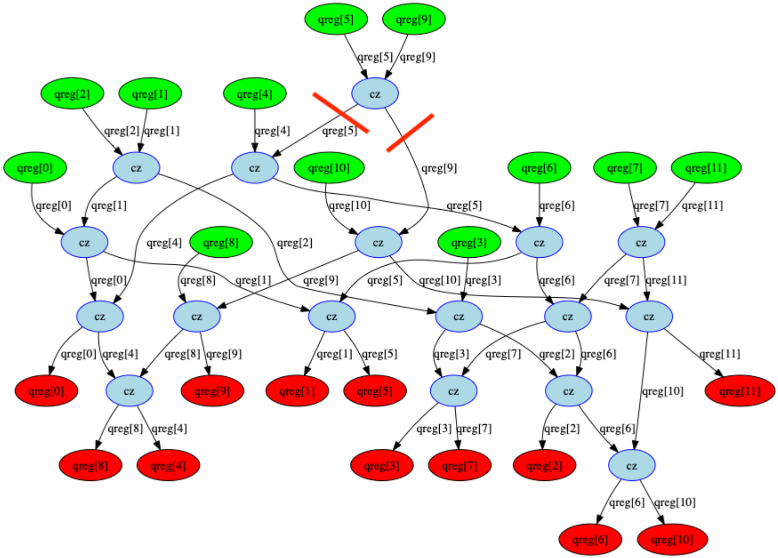


Highlights the need for specialized optimization methods for quantum variational algorithms

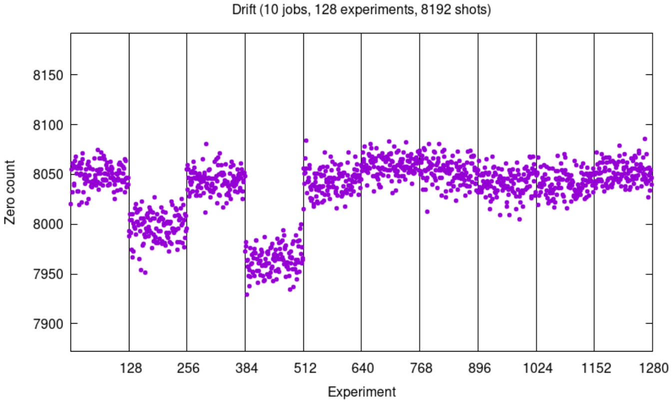
Cutting quantum circuits



Cutting quantum circuits



Control of time-varying systems



Experiment on qubit 0 of an IBM 20-qubit chip obtained on 3/23/19